NanoElectronic MOdeling (NEMO)

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The design of resonant tunneling based quantum devices requires accurate modeling of the quantum charge, resonant levels, and scattering effects in extremely complicated and varied potential profiles made possible by the great flexibility of hetero-epitaxial based band engineering. Until now, such a device simulator did not exist. We unveil an alpha version of such a tool. It is planned for this tool to become available to the national R&D community.

The tool solves the non-equilibrium Green function equations including realistic models for the important scattering mechanisms: polar-optical phonon, acoustic phonon, alloy, and interface roughness. Novel boundary conditions allow us to treat large sections of the leads via boundary conditions even when the leads have spatially varying potentials. This enables us to model very long devices, and it allows us to model injection into the device from quantized states in the emitter. The simulator was run against an extensive test matrix of in-house experimental data and was found to show good agreement both qualitatively and quantitatively. We are incorporating into the code a general multi-band platform which presently includes the following models: coupled one-band model (Liu), discretized 2 and 4 band models (Kane), 2nd nearest neighbor sp^3 (Slater), and nearest neighbor sp^3s^* (Vogl). Results of multi-band calculations will be discussed.

We show the impact of different scattering mechanisms on the valley current of an $In_{0.53}Ga_{0.47}As$ / $In_{0.52}Al_{0.48}As$ resonant tunneling diode (RTD) with asymmetric roughness of the interfaces. Based on STM measurements, we let the first and third interfaces from the emitter be rough with an average island size of 12 nm with the second and fourth interfaces smooth. In the forward bias direction, the interface roughness scattering dominates the valley current, while in the reverse bias direction (rough interfaces on the second and fourth interfaces from the emitter) the polar optical phonon scattering dominates the valley current.

We explore the utility and accuracy of our novel boundary conditions by modeling an experimental GaAs / $Al_{0.4}Ga_{0.6}As$ RTD[1] and an Opto-RTD[2] and quantitatively show that the structure in the turn-on of the I-V is a result of the quantized states in the emitter interacting with the resonant state in the well. We also show the importance of treating scattering in the leads.

We consider the design of a triple barrier $In_{0.53}Ga_{0.47}As$ / AlAs structure to obtain an I-V with two consecutive peaks of equal height with good peak to valley ratios. We first turn off the scattering for fast turn-around and find a structure that satisfies the above criteria. Then we investigate the effects of scattering. Alloy, acoustic phonon and polar optical phonon scattering have little effect on the first peak while interface roughness scattering reduces the magnitude of the peak by a factor of ten. Unlike double barrier RTD's, certain triple barrier structures require a treatment of scattering to obtain, even qualitatively, the correct resonant current.

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[1] J. Wu *et al.*, *Sol. State Elect.*, **34**, 403 (1991). See Figs. (2d) and (10).
[2] T. Moise, 52nd Annual Device Research Conference Digest, p. VA-4.

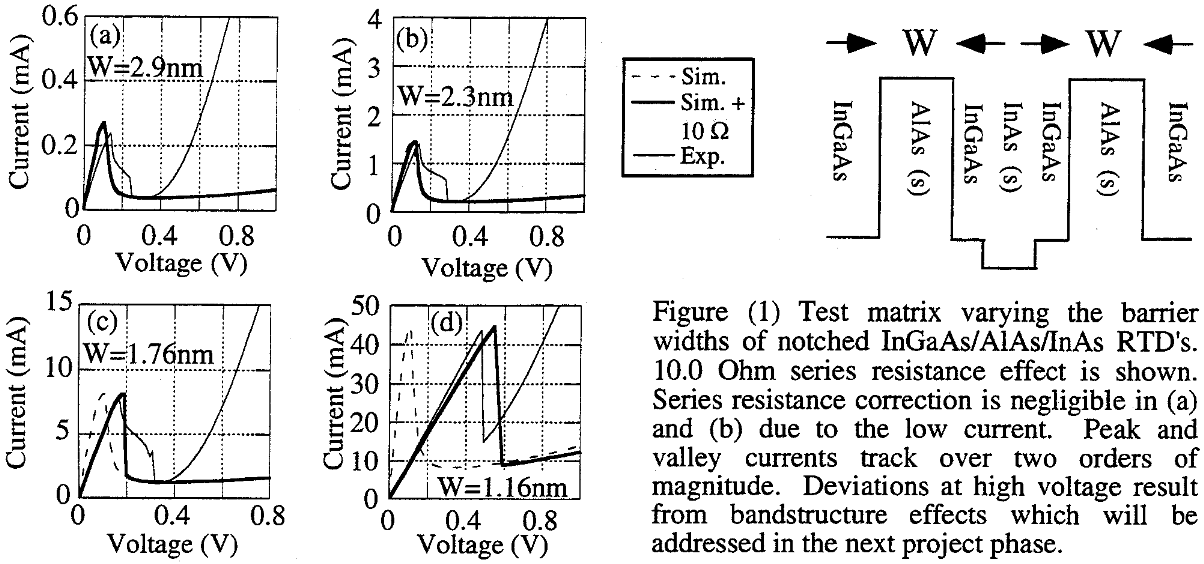

Figure (1) Test matrix varying the barrier widths of notched InGaAs/AlAs/InAs RTD's. 10.0 Ohm series resistance effect is shown. Series resistance correction is negligible in (a) and (b) due to the low current. Peak and valley currents track over two orders of magnitude. Deviations at high voltage result from bandstructure effects which will be addressed in the next project phase.

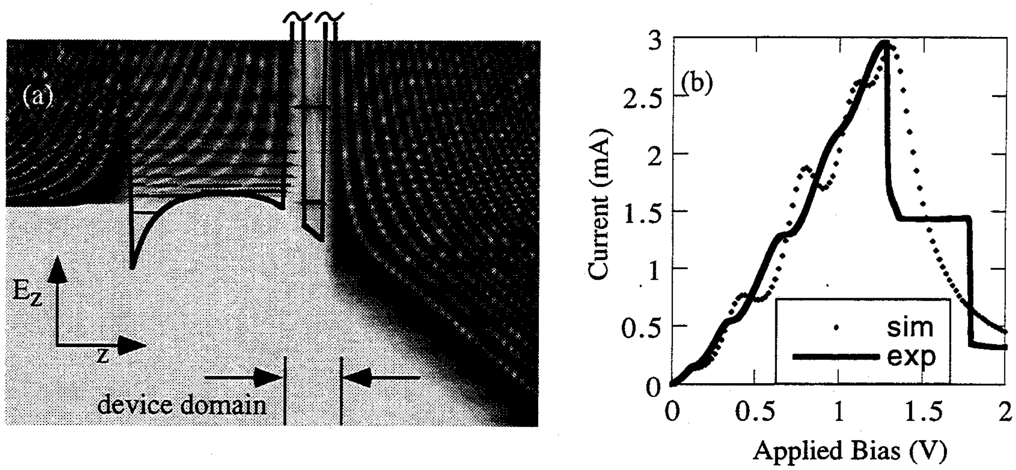

Figure (2) Opto-RTD simulation. Novel boundary conditions account for injection from quantized emitter states. (a) Local density of states with superposed conduction band profile. Dark regions correspond to a high density of states. Multiple quantized emitter states are evident. Non-equilibrium transport is calculated in the device domain only (see label in figure). States in the region outside that domain are treated by novel boundary conditions. (b) Simulated and experimental I-V curves. No scattering was included in the device domain.

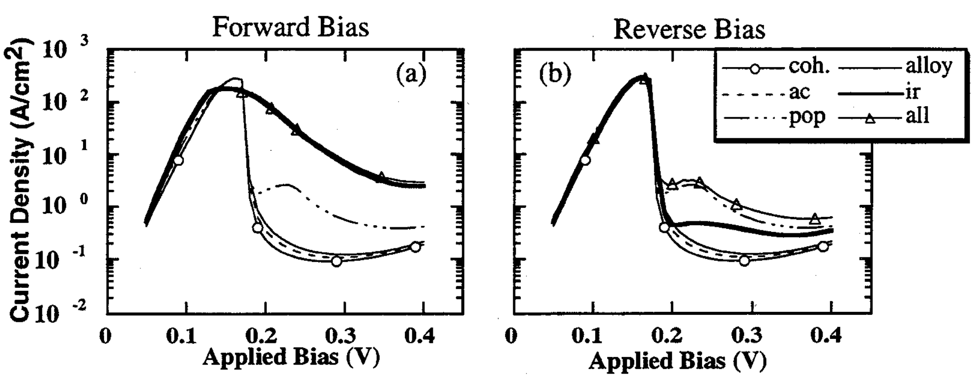

Figure (3) Simulated I-V of an InGaAs/InAlAs RTD with asymmetric roughness of the interfaces at 77K. Different scattering mechanisms are simulated individually to show their relative importance. (a) In forward bias, the first and third interfaces from the emitter are rough and the other two are smooth. Interface roughness is the dominating scattering mechanism. (b) In reverse bias, polar optical phonon scattering is the dominant scattering mechanism.